

Acetic acid, trifluoro-, methyl ester
431-47-0 | DTXSID2059988

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.24

Global applicability domain: Inside

Local applicability domain index: 3.90e-01

Confidence level: 9.06e-01

Nearest Neighbors from the Training Set

Image not found

Sulfolane

Measured: 7.08

Predicted: 6.91

Image not found

2,2-Dimethylpropane-1,3-diol

Measured: 4.68

Predicted: 4.44

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tert-Butyl alcohol

Measured: 5.01

Predicted: 4.48

Image not found

Thiourea

Measured: 2.00

Predicted: 2.11

Image not found

Dimethyl sulfoxide

Measured: 3.98

Predicted: 4.07